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The Harmonic Oscillator, The Hermite Polynomial Solutions

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I. SYNOPSIS

The Harmonic Oscillator's Quantum Mechanical solution involves Hermite Polynomials, which are introduced here in various guises any one of which the reader may find useful as a starting points.

II. WRITING THE SCHRÖDINGER EQUATION IN DIMENSIONLESS FORM

The relevant Schrödinger Equation is

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}\psi + \frac{k}{2}z^2\psi = E\psi \tag{2.1}$$

where k is the force constant (dynes/cm) and μ is the reduced mass (grams). Cross multiplying, one has

$$\frac{\partial^2}{\partial z^2}\psi - \frac{k\mu}{\hbar^2}z^2\psi = -\frac{2\mu}{\hbar^2}E\psi \tag{2.2}$$

which would be simplified if the constants could be suppressed. To do this we change variable, from z to something else, say x, where $z = \alpha x$. Then

$$\frac{\partial}{\partial z} = \frac{\partial x}{\partial z}\frac{\partial}{\partial x} = \frac{1}{\alpha}\frac{\partial}{\partial x}$$

so

$$\left(\frac{1}{\alpha^2}\right)\frac{\partial^2}{\partial x^2}\psi - \frac{k\mu}{\hbar^2}\alpha^2 x^2\psi = -\frac{2\mu}{\hbar^2}E\psi \tag{2.3}$$

and

$$\frac{\partial^2}{\partial x^2}\psi - \frac{k\mu}{\hbar^2}\alpha^4 x^2\psi = -\alpha^2\frac{2\mu}{\hbar^2}E\psi \tag{2.4}$$

which demands that we treat

$$1 = \frac{k\mu}{\hbar^2}\alpha^4$$

$$\alpha = \left(\frac{1}{\frac{k\mu}{\hbar^2}}\right)^{1/4} = \left(\frac{\hbar^2}{k\mu}\right)^{1/4}$$

With this choice, the differential equation becomes

$$\frac{\partial^2\psi}{\partial x^2} - x^2\psi = -\epsilon\psi \tag{2.5}$$

where

$$\epsilon = \frac{2\alpha^2\mu E}{\hbar^2} = \frac{2\sqrt{\frac{\hbar^2}{k\mu}}\mu E}{\hbar^2} = \frac{2E\sqrt{\frac{\mu}{k}}}{\hbar}$$

III. GUESSWORK FOR THE GROUND STATE

The easiest solution to this differential equation is

$$e^{-\frac{x^2}{2}}$$

which leads to

$$E = \frac{\hbar}{2}\sqrt{\frac{k}{\mu}}$$

IV. A GENERATING FUNCTION SCHEME

Given

$$\psi_0 = |0> = e^{-\frac{x^2}{2}}$$

with $\epsilon = 1$, it is possible to generate the next solution by using

$$N^+ = -\frac{\partial}{\partial x} + x \tag{4.1}$$

as an operator, which ladders up from the ground (n=0) state to the next one (n=1) To see this we apply N^+ to ψ_0 obtaining

$$N^+\psi_0 = N^+|0> = \left(-\frac{\partial}{\partial x} + x\right)e^{-\frac{x^2}{2}} = -(-x)\psi_0 + x\psi_0 = 2xe^{-x^2/2} = \psi_1 = |1> \tag{4.2}$$

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Doing this operation again, one has

$$N^+\psi_1 = N^+|1>= \left(-\frac{\partial}{\partial x}+x\right)2xe^{-\frac{x^2}{2}} = (-2+4x^2)e^{-x^2/2} \tag{4.3}$$

etc., etc., etc..

V. HERMITE POLYNOMIAL DEFINITION

Assuming

$$\psi = e^{-x^2/2}H(x)$$

where H(x) is going to become a Hermite polynomial. One then has

$$\frac{d\psi}{dx} = -xe^{-x^2/2}H(x) + e^{-x^2/2}\frac{dH(x)}{dx}$$

and

$$\frac{d^2\psi}{dx^2} = -e^{-x^2/2}H(x) + x^2e^{-x^2/2}H(x) - 2xe^{-x^2/2}\frac{dH(x)}{dx} + e^{-x^2/2}\frac{d^2H(x)}{dx^2}$$

From Equation 2.5 one has,

$$\frac{\partial^2\psi}{\partial x^2} - x^2\psi = -e^{-x^2/2}H(x) - 2xe^{-x^2/2}\frac{dH(x)}{dx} + e^{-x^2/2}\frac{d^2H(x)}{dx^2} = -\epsilon e^{-x^2/2}H(x) \tag{5.1}$$

or

$$-H(x) - 2x\frac{dH(x)}{dx} + \frac{d^2H(x)}{dx^2} = -\epsilon H(x) \tag{5.2}$$

which we re-write in normal lexicographical order

$$\frac{d^2H(x)}{dx^2} - 2x\frac{dH(x)}{dx} - (1-\epsilon)H(x) = 0 \tag{5.3}$$

This is Hermite's differential equation.

VI. GENERATING HERMITE'S DIFFERENTIAL EQUATION

Starting with

$$\frac{dy}{dx} + 2xy = 0 \tag{6.1}$$

one has

$$\frac{dy}{y} = -2xdx$$

so, integrating each side separately, one has

$$\ell ny = -x^2 + \ell nC$$

or, inverting the logarithm,

$$y = Ce^{-x^2}$$

We now differentiate Equation 6.1, obtaining

$$\frac{d^2y}{dx^2} + 2\frac{d(xy)}{dx} = \frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + 2y\frac{dx}{dx} = \frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + 2y = 0\,;\, n=0 \tag{6.2}$$

Doing this again, i.e., differentiating this (second) equation (Equation 6.2), one has

$$\frac{d\frac{d^2y}{dx^2}}{dx} + \frac{d2x\frac{d(y)}{dx}}{dx} + 2\frac{dy}{dx} = \frac{d^2\left(\frac{dy}{dx}\right)}{dx^2} + 2x\frac{d\left(\frac{dy}{dx}\right)}{dx} + 4\left(\frac{dy}{dx}\right) = 0\,;\, n=1$$

which is the same equation, (but with a 4 multiplier of the last term) applied to the first derivative of y. Take the derivative again:

$$\frac{d\left(\frac{d^2\frac{dy}{dx}}{dx^2}+2x\frac{d\frac{dy}{dx}}{dx}+4\frac{dy}{dx}\right)}{dx}=0$$

i.e.,

$$\frac{d^2\left(\frac{d^2y}{dx^2}\right)}{dx^2}+2x\frac{d\left(\frac{d^2y}{dx^2}\right)}{dx}+6\left(\frac{d^2y}{dx^2}\right)=0$$

$$\frac{d^2f(x)}{dx^2}+2x\frac{df(x)}{dx}+6f(x)=0\,;\;n=2$$

f(x) has the form $g(x)e^{-x^2}$ where g(x) is a polynomial in x.

$$\frac{d^2g(x)e^{-x^2}}{dx^2}+2x\frac{dg(x)e^{-x^2}}{dx}+2(n+1)g(x)e^{-x^2}=0$$

i.e.,

$$\left(g''(x)-4xg'(x)-2g(x)+4x^2g(x)+2xg'(x)-4x^2g(x)+2(n+1)g(x)\right)e^{-x^2}=0$$

or

$$g''(x)-2xg'(x)+2ng(x)=0$$

and we had

$$H''(x)-2xH'(x)-(1-\epsilon)H(x)=0$$

which leads to

$$2n=-1+\epsilon$$

i.e.,

$$\epsilon=1+2n=\frac{2E\sqrt{\mu/k}}{\hbar}$$

i.e.,

$$E=\hbar(n+\frac{1}{2})\sqrt{\frac{k}{\mu}}$$

VII. FROBENIUS, BRUTE FORCE, METHODOLOGY

The most straight forward technique for handling the Hermite differential equation is the method of Frobenius. We assume a power series *Ansatz* (ignoring the indicial equation argument here), i.e.,

$$\psi=\sum_{i=0}a_ix^i$$

and substitute this into Equation 5.3, obtaining

$$\frac{\partial^2\psi}{\partial x^2}=\sum_{i=2}i(i-1)a_ix^{i-2}$$
$$-2x\frac{\partial\psi}{\partial x}=-2\sum_{i=1}ia_ix^i$$
$$(\epsilon-1)\psi=(\epsilon-1)\sum_i a_ix^i=0$$

i.e.,

$$\frac{\partial^2\psi}{\partial x^2}=2(1)a_2+(3)(2)a_3x+(4)(3)a_4x^2+\cdots$$
$$-2x\frac{\partial\psi}{\partial x}=-2a_1x^1-2a_2x^2-2a_3x^3-\cdots$$
$$(\epsilon-1)\psi=(\epsilon-1)a_0+(\epsilon-1)a_1x+(\epsilon-1)a_2x^2-\cdots=0$$

which leads to

$$(2)(1)a_2+(\epsilon-1)a_0=0\;(even)$$

$$(3)(2)a_3+(\epsilon-1)a_1-2a_1=0\;(odd)$$

$$(4)(3)a_4-2a_2+(\epsilon-1)a_2=0\;(even)$$

$$(5)(4)a_5-2a_3+(\epsilon-1)a_3=0\;(odd)$$

which shows a clear division between the even and the odd powers of x. We can solve these equations sequentially.

We obtain

$$a_2=\frac{1-\epsilon}{(2)(1)}$$

$$a_3=\frac{2+1-\epsilon}{(3)(2)}a_1$$

$$a_4=\frac{2+1-\epsilon}{(4)(3)}a_2=\left(\frac{2+1-\epsilon}{(4)(3)}\right)\left(\frac{1-\epsilon}{(2)(1)}\right)$$

i.e.,

$$a_4=\left(\frac{(3-\epsilon)(1-\epsilon)}{(4)(3)(2)(1)}\right)$$

etc..

This set of even (or odd) coefficients leads to a series which itself converges unto a function which grows to positive infinity as x varies, leading one to require that the series be terminated, becoming a polynomial.

We leave the rest to you and your textbook.